Homogenization in three-dimensional phononic crystals

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Homogenization in three-dimensional phononic crystals

R Sainidou

Instituto de Óptica, CSIC, Serrano 121, 28006, Madrid, Spain.

E-mail: `rsainid@io.cfmac.csic.es`

Abstract. We use a simple model to determine the frequency-dependent effective elastic coefficients of a three-dimensional phononic crystal, consisting of periodically arranged solid spheres embedded in fluid host, through theoretical calculations of the transmission coefficient and frequency band structure diagrams, using multiple-scattering techniques. Our results are successfully compared to those obtained from effective medium theories at the long wavelength limit.

1. Introduction

Phononic crystals are composite materials consisting in the simplest case of a periodic arrangement of cylindrical or spherical inclusions (two- or three-dimensional case, respectively) characterized by elastic coefficients (the mass density, ρ_s, and the longitudinal and transverse velocities of propagation of elastic waves, $c_{l\mathrm{s}}$ and $c_{t\mathrm{s}}$, respectively) and embedded in a host matrix of different elastic coefficients. Over the last years the problem of homogenization, i.e. the description of this composite system by a unique set of elastic parameters, has attracted a lot of attention [1–4]. However, the relevant results refer mostly to the long-wavelength limit ($\omega \to 0$) [1–3] and/or they cannot predict all of the three parameters [4]. In this work we deal with three-dimensional phononic crystals and we focus for simplicity on the case of solid spheres in a fluid host matrix. We use a simple model to determine the frequency-dependent effective elastic coefficients of such a system, through theoretical calculations of the transmission coefficient and frequency band structure diagrams, using multiple-scattering techniques [5]. Several filling fractions are considered and the possibility of a successful and coherent physical description of the system under consideration, via the proposed homogenization, is discussed.

2. Results and discussion

We consider a fcc crystal, of lattice constant $a_0\sqrt{2}$ (a_0 is the first-neighbour distance), consisting of steel spheres (mass density: $\rho_\mathrm{s} = 7800$ kg/m^3, longitudinal and transverse velocities: $c_{l\mathrm{s}} = 5940$ m/s and $c_{t\mathrm{s}} = 3200$ m/s) in water (mass density: $\rho_{water} = 1000$ kg/m^3, sound velocity: $c_{water} = 1480$ m/s). The spheres have radius $S = 0.48a_0$, leading to a value $f = \frac{4\pi\sqrt{2}}{3}(S/a_0)^3 = 0.65$ for the volume filling fraction of the crystal.

For the homogenization of the composite system within a frequency range and not only at the long wavelength limit ($\omega \to 0$), one needs to make the assumption that for any frequency ω this system in its finite form (i.e. a slab of the above crystal constructed as a sequence of

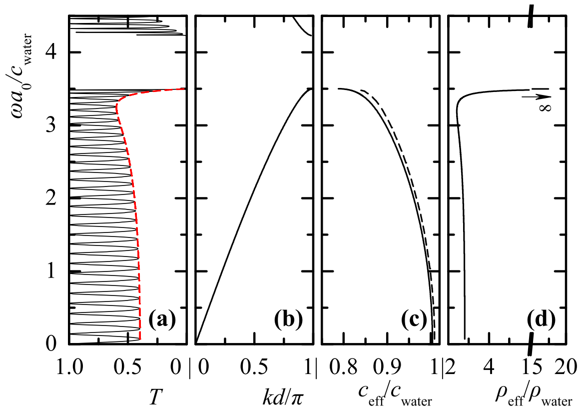

Figure 1. (a) Transmission spectrum for a longitudinal acoustic wave incident normally on a slab of 32 fcc (001) layers of steel spheres (radius $S = 0.48a_0$, a_0: first-neighbour distance) in water. Red dashed line: the envelope of transmission minima. (b) The phononic band structure of the corresponding infinite crystal, along the [001] direction. (c) The effective velocity as calculated from the first band in the dispersion plot (b) through Eq. (3) (solid line), and from the transmission spectrum (a) through Eqs. (4) (dashed line). (d) The corresponding effective mass density, obtained by Eq. (4).

$N_{\rm L}$ successive layers of spheres with a distance d between them) is equivalent to a homogeneous slab of the same thickness $D = N_{\rm L}d$, whose elastic parameters (mass density and elastic wave velocities) are in the general case frequency-dependent: $\rho_{\rm eff}(\omega)$, $c_{\rm eff}(\omega)$. The transmittance T of such a homogeneous (effective) slab, sandwiched on both sides by a fluid infinite medium (characterized by ρ_h, c_h), when a longitudinal plane wave of frequency ω is incident normally on it, is given by [6]

$$T(\omega) = \frac{4\zeta^2}{(1+\zeta^2)^2 - (1-\zeta^2)^2\cos^2\phi} \, , \tag{1}$$

where $\zeta(\omega) = \frac{c_h}{c_{\rm eff}}\frac{\rho_h}{\rho_{\rm eff}}$ and $\phi(\omega) = \omega D/c_{\rm eff}$. In the case considered here $\rho_h = \rho_{\rm water}$ and $c_h = c_{\rm water}$. The key for the determination of the effective elastic parameters is the detailed form of the transmission spectrum together with the band structure of the corresponding infinite system. In Fig. 1(a) we show the transmission spectrum of a longitudinal acoustic wave incident normally on a sufficiently thick finite slab of this crystal, constructed as a sequence of $N_{\rm L} = 32$ successive (001) fcc planes of spheres (layers), with a distance $d = a_0\sqrt{2}/2$ between them. Next to it, we present the corresponding band structure, along the [001] (i.e. ΓX) direction, which we calculated using the computer program of Ref. [5]. The most important characteristic of the transmittance for a sufficiently thick slab is the appearance of numerous Fabry-Perot-type-like oscillations, whose number depends on N_L, between the unity (maxima occurring at ω_M, when $\cos\phi = 1$) and an envelope function (minimum value occurring at ω_m, when $\cos\phi = 0$). This leads to the following conditions

$$\begin{aligned} \phi_n(\omega_M) \equiv \omega_M D/c_{\rm eff} = n\pi, \; n = 0, 1, \cdots, N_L - 1, \\ \phi_n(\omega_m) \equiv \omega_m D/c_{\rm eff} = (n + 1/2)\pi, \; n = 0, 1, \cdots, N_L - 2. \end{aligned} \tag{2}$$

from which the effective velocity $c_{\rm eff}(\omega)$ can be determined (the values ω_M, ω_m are known from the transmission spectrum), since ζ changes with ω much slower than ϕ does. This is shown in Fig. 1(c), together with the effective velocity, as obtained from the first band in the band structure plot [Fig. 1(b)]

$$c_{\rm eff}(\omega) = \omega(k)/k \, . \tag{3}$$

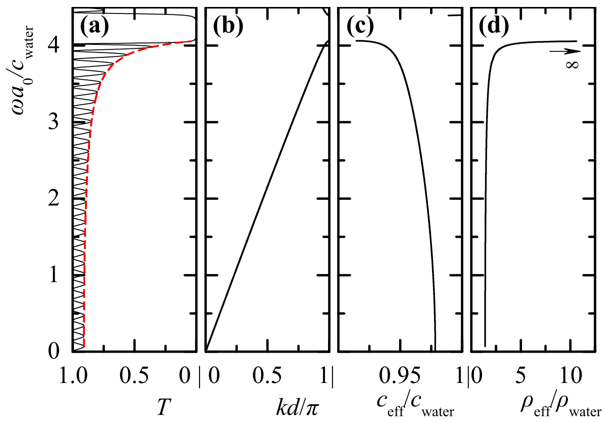

Figure 2. (a) Transmission spectrum for a longitudinal acoustic wave incident normally on a slab of 32 fcc (001) layers of steel spheres (radius $S = 0.35a_0$, a_0: first-neighbour distance) in water. Red dashed line: the envelope of transmission minima. (b) The phononic band structure of the corresponding infinite crystal, along the [001] direction. (c) The effective velocity as calculated from the first band in the dispersion plot (b), through Eq. (3). (d) The corresponding effective mass density, obtained by Eq. (4).

The small difference in the two curves is due to the size of the slab: for a thicker one (N_L=128) the effective velocity curve obtained by the transmission through Eqs. (2) [dashed line in Fig. 1(c)] coincides with those obtained from the band structure [solid line in Fig. 1(c)]. A similar procedure based only on the first of Eqs. (2) has already been used in the case of two-dimensional phononic crystals [4], however the information of minima were not included in the above analysis. Here we show that the minima can successfully reproduce the effective velocity curve as obtained from the band structure calculation, and more importantly, the minima envelope function in the transmission [red dashed line in Fig. 1(a)] can provide us with a tool to determine the effective mass density, $\rho_{\rm eff}$, as follows. For the points lying on the envelope, we have $\cos\phi = 0$, and from Eq. (1) this results to $\tau_m \equiv T(\omega_m) = 4\zeta^2/(1+\zeta^2)^2$. The latter leads to

$$\frac{\rho_{\rm eff}(\omega)}{\rho_h} = \left(\frac{c_{\rm eff}(\omega)}{c_h}\right)^{-1} \frac{\sqrt{\tau_m}}{1-\sqrt{1-\tau_m}}\ , \tag{4}$$

with τ_m depending of course on ω. This is shown in Fig. 1(d). A general remark to be made is that the effective mass density follows the shape of the minima envelope of the transmission spectrum. This shape changes by changing the size of the spheres (i.e. the volume filling fraction f of the infinite crystal). As an example we give in Fig. 2 the corresponding to Fig. 1 case, for $S = 0.35a_0$. One clearly sees that the envelope is now a monotonically decreasing function of frequency, whose value away from the end of the band increases for smaller spheres. It is also worth noting that at the upper frequency limit of the first band, ω_u, the envelope goes to zero, therefore $\rho_{\rm eff}$ diverges at this limit. This is consistent with the existence of the gap region: it is like if the system behaves as an impenetrable object, because of the destructive interference of the multiple scattering on the periodic array.

In Fig. 3 we show the dependence of the effective parameters on the filling fraction for the whole frequency region where the first band extends. The values of the elastic parameters at the long wavelength limit ($\omega \to 0$), as calculated from the method presented here, fulfill the isotropy condition (we obtain the same results for ΓL direction) and are in very good agreement

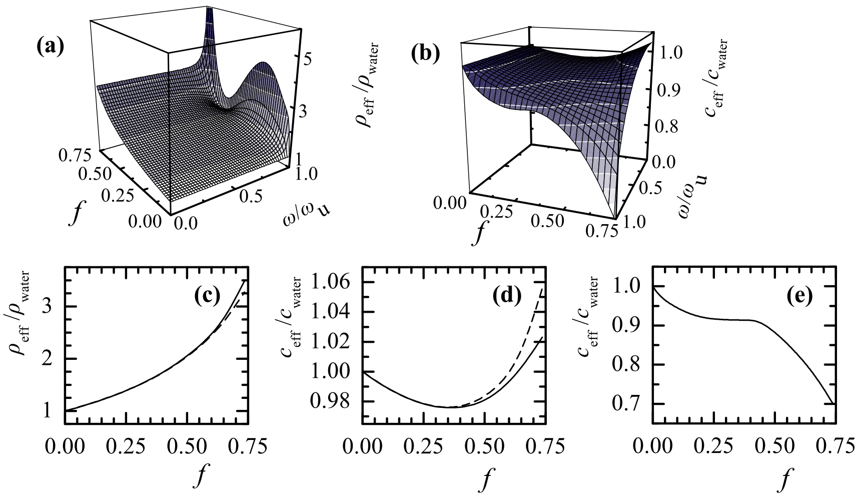

Figure 3. The effective mass density (a) and the effective velocity (b) as a function of frequency and filling fraction, calculated from Eqs. (4), (3). In (c), (d) detail of (a), (b) at the long wavelength limit (solid line) together with the results of Eqs. (5), (6) (dashed line). (e) The effective velocity calculated from Eq. (3) at the upper frequency limit, ω_u, of the band.

with those calculated from other (static) effective medium theories [7] through the equations

$$\frac{\rho_{\rm eff}}{\rho_h} = \frac{1-f+\frac{\rho_{\rm s}}{\rho_h}(2+f)}{1+2f+2\frac{\rho_{\rm s}}{\rho_h}(1-f)} \tag{5}$$

and

$$\frac{c_{\rm eff}}{c_h} = \left\{\frac{\rho_{\rm eff}}{\rho_h}\left[1-f+f\frac{\rho_h}{\rho_{\rm s}}\left[\left(\frac{c_{l\rm s}}{c_h}\right)^2-\frac{4}{3}\left(\frac{c_{t\rm s}}{c_h}\right)^2\right]^{-1}\right]\right\}^{-1/2} . \tag{6}$$

The comparison is shown in Figs. 3(c),(d) together with the effective velocity curve at the upper band limit, ω_u [Fig. 3(e)].

3. Conclusions

In this work we presented a simple model to determine the frequency-dependent effective elastic coefficients of a fcc phononic crystal of steel spheres immersed in water, successfully compared to those obtained from effective medium theories at the long wavelength limit. This study, limited here within the first band region and for the case of normal incidence of a longitudinal wave on a finite slab of such a crystal, could be extended to frequency regions within gaps and higher bands and for oblique incidence (in which case the extension should be made with care, since the propagation in the long-wavelength region is forbidden).

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